# A Local Minimax-Newton Method for Finding Multiple Saddle Points with Symmetries

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**Abstract**

In this paper, a local minimax-Newton method is developed to solve for multiple saddle points. The local minimax method [15] is used to locate an initial guess and a version of the generalized Newton method is used to speed up convergence. When a problem possesses a symmetry, the local minimax method is invariant to the symmetry. Thus the symmetry can be used to greatly enhance the efficiency and stability of the local minimax method. But such an invariance is sensitive to numerical error and the Haar projection has been used to enforce the symmetry [27]. In this paper, we prove that the Newton method is invariant to symmetries and that such an invariance is insensitive to numerical error. When a symmetric degeneracy takes place, it is proved that the Newton direction can be easily solved in an invariant subspace. Thus the Newton method can be used not only to speed up convergence but also to avoid using the Haar projection if the symmetric degeneracy is removable by a discretization. Finally, numerical examples are presented to illustrate the theory.

**Keywords**. Saddle point, Symmetry, Group action, Invariance, Newton's method

**AMS(MOS) subject classifications**. 35A40,35A15,58E05,58E30

**Abbreviated titles**. A Local Minimax-Newton Method

# 1 Introduction

Let $H$ be a Hilbert space with inner product $\langle \cdot, \cdot \rangle$ and $J \in C^2(H, \mathbb{R})$, $J' : H \to H^*$ be its Frechet derivative and $\nabla J : H \to H$ be the gradient, and $J'' : H \to L(H, H^*)$ its second

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Frechet derivative. Since there is a canonical identification between $H^*$ and $H$, $\nabla J(u)$ is the identification of $J'(u)$. We may also use the identification of $J''(u)$ so $J''(u)$ is seen as in $L(H,H)$. A point $u \in H$ is a critical point of $J$ if $u$ solves the Euler-Lagrange equation $J'(u) = 0$. Many boundary value problems in nonlinear elliptic PDEs can be converted to solving its Euler-Lagrange equation for a critical point. A critical point $u$ is non-degenerate if $J''(u)$ is invertible. The first candidates for a critical point are the local extrema which are well-studied in the classical calculus of variation. Traditional numerical (variational) methods focus on finding such stable solutions. Critical points that are not local extrema are *unstable* and called *saddle points*. In physical systems, saddle points appear as unstable equilibria or transient excited states. A huge number of papers exist in the literature on the existence of multiple saddle points in various nonlinear problems.

To theoretical and computational physics and chemistry, saddle points between two stable states on the potential hypersurface are of great interests and lie in the theme of so called Transition State Theory or Activated Complex Theory, as they correspond to the transition states or the minimum energy paths between reactant molecules and product molecules [13]. A large literature can be found in this area.

Solitons arise in many fields, such as condensed matter physics, dynamics of biomolecules, nonlinear optics, etc. Among them, solutions which are not ground states, are the so-called excited states. In the study of self-guided light waves in nonlinear optics [11,12,19], excited states are of great interests. All those solitons are saddle points, thus unstable solutions.

On the other hand, symmetries exist in many natural phenomena, such as in crystals, elementary particle physics, symmetry of the Schrödinger equation for the atomic nucleus and the electron shell with respect to permutations and rotations, energy conservation law for systems which are invariant w.r.t. time translation, etc. Symmetries described by compact group actions in variational problems have been used in the literature to prove the existence of *multiple critical points*, typically, in the Ljusternik-Schnirelman theory (see, e.g., [14] and others). It is known that symmetries in a nonlinear variational problem can lead to the existence of many solutions of saddle type and can also cause (symmetric) degeneracy.

Due to the unstable nature, finding multiple saddle points numerically *in a stable way* is very challenging. There is virtually no theory in the literature to devise such a numerical algorithm until recently a local minimax method was developed in [15,16] to find multiple saddle points in a sequential order of their Morse indices and its convergence was established in [16]. Techniques to enhance efficiency and stability of this method for computing saddle points with symmetries by using the Haar projection are developed in [27].

Since the local minimax method [15,16] is a gradient type, first order algorithm, to speed up convergence, it is quite natural to consider a Newton's method. Due to the instability and multiplicity nature of our problems, we consider a Newton's method of the form

$$u_{k+1} = u_k - s_k \nu_k \quad \text{with} \quad \nu_k = (J''(u_k))^{-1} J'(u_k)$$

where $\nu_k$ is the Newton direction and $s_k > 0$ is a stepsize to enhance the stability of the algorithm, e.g., in Armijo's rule, $s_k > 0$ is chosen such that

$$\|\nabla J(u_{k+1})\| - \|\nabla J(u_k)\| < -\frac{1}{2} s_k \|\nabla J(u_k)\|. \tag{1.1}$$

For the algorithm to converge to a desirable critical point, two basic conditions are assumed:
(a) a good initial guess to start with, otherwise it can be extremely slow or divergent, or can lead to an unwanted trivial or known critical point;
(b) the problem has to be nondegenerate, i.e., $J''(u_k)$ is invertible along the trajectory of a Newton's method.

When $J''(u_k)$ is not invertible, a generalized Newton's method is suggested in the literature by using the generalized (Moore-Penrose) inverse $J''(u_k)^\dagger$, where the Newton direction $\nu_k = J''(u_k)^\dagger J'(u_k)$ is the least-norm solution to the minimization problem

$$\min_{\nu \in H} \|J''(u_k)\nu - J'(u_k)\|. \tag{1.2}$$

Under standard conditions and $s_k \equiv 1$, the generalized Newton method converges locally and quadratically [20]. This approach seems to be very general but also too complicated to apply to solve an infinite-dimensional problem. Therefore people tend to avoid using the generalized Newton method in solving variational problems. It is also very difficult for us to examine its response to the effects of a symmetry in a problem.

Although attempts have been made by several researchers, e.g., [18, 22] to use a Newton's method to find multiple saddle points in various problems, the question on how to deal with those two basic conditions (a) and (b) remains unanswered. Locating a good initial guess in an infinite-dimensional space is itself a challenging problem, in particular, when multiple solutions are involved. By using the local minimax method [15, 16], a good initial guess can be provided. However, degeneracy exists in every multiple saddle point problem due to a sign change of the eigenvalues of $J''(u)$. Either a solution to be found is degenerate or $J''(u)$ is not invertible at a point $u$ along the Newton trajectory. How to handle such a case within the framework of a Newton's method remains to be a very interesting problem. On the other hand, when the problems possess some symmetries, they may create symmetric degeneracy, see Example 2.1. How a Newton's method responds to symmetries of the problems is, in general, still unknown. In this paper we shall try to address these questions. To do so, we use an approach somewhat between the standard and the generalized Newton method. When $J$ is $C^2$ and $J''(u)$ has a closed range, for given $u \in H$, we consider a solution $\nu$ to

$$J''(u)\nu = J'(u). \tag{1.3}$$

In the following we assume that $J''(u)$ is a Fredholm operator with index zero. Since $J''(u)$ is self-adjoint, it has a finite dimensional kernel, $\ker(J''(u))$ and a closed range. Then it is known that (1.3) may have none, unique or infinitely many solutions, and (1.3) has a solution if and only if $\nabla J(u) \perp \ker(J''(u))$. In this case, *the Newton direction is just the least-norm solution* to the linear system (1.3). Note that in general, with the Armijo rule (1.1), the Newton method may approximate a critical point $u^*$ of the function $g(u) = \|\nabla J(u)\|$, i.e.,

$$\langle g'(u^*), v\rangle = \frac{\langle J''(u^*)v, \nabla J(u^*)\rangle}{\|\nabla J(u^*)\|} = 0, \quad \forall v \in H.$$

If we choose $v = \nu$, a solution to (1.3), we have $J''(u^*)\nu = \nabla J(u^*)$ and $\langle g'(u^*), \nu\rangle = \|\nabla J(u^*)\| = 0$. Thus a critical point $u^*$ of $g(u) = \|\nabla J(u)\|$ where (1.3) is solvable must be a critical point of $J$.

In this paper, we assume that a solution $u^*$ to be found possesses certain symmetry and that the degeneracy of $u^*$ is created *only* by the symmetry. Our method will be particularly useful in situations where there are multiple saddle point type solutions due to symmetries. Our analysis uncovers the effects of symmetries in the problems on the Newton method. In summery, we shall undertake the following steps towards giving a theoretical strategy and implementing a numerical algorithm for computing multiple saddle point type solutions when symmetry is at present:

(1) prove the invariance of the Newton direction under symmetries;

(2) prove the solvability of (1.3) under symmetric degeneracies;

(3) show that the invariance of the Newton direction to symmetries is insensitive to numerical error, which contrasts to the fact that the invariance of the local minimax method to symmetries is sensitive to numerical error [27].

Due to the invariance of the local minimax method to symmetries, symmetries can be used to greatly enhance the efficiency and stability of the method [27]. However, such an invariance is sensitive to numerical error. Thus the Haar projection has to be used to enforce the symmetry. When a symmetry is associated with a continuous group of actions, the corresponding Haar projection is an integral over the group. It becomes very difficult to compute. On the other hand, in many applications such as those examples in this paper, such a symmetric degeneracy is removable when a discretization of the problem is used. After the analysis in this paper we realize that with a least-norm solution linear solver, the Newton method can be used, following the local minimax method, to not only speed up convergence but also avoid using the Haar projection when the symmetric degeneracy is removable by a discretization. This is *the local minimax-Newton method* we shall describe in this paper. In the last section, we present several numerical examples to illustrate the theory.

# 2 The Newton Method

Let $H$ be a Hilbert space, $\mathcal{G}$ be a compact Lie group that acts isometrically on $H$ and $J \in C^2(H, \mathbb{R})$ be $\mathcal{G}$-invariant, i.e., $J(gu) = J(u),\ \forall g \in \mathcal{G}, u \in H$, and $J''(u)$ have a closed range for each $u \in H$. For a subgroup $G$ of $\mathcal{G}$, let $H_G = \{u \in H \mid gu = u, \forall g \in G\}$ be the invariant subspace of $H$ under the group actions of $G$. For $u \in H$, the G-orbit of $u$ is the set $Gu = \{gu : g \in G\}$ and the isotropy subgroup of $u$ is $\mathcal{G}_u = \{g \in \mathcal{G} : gu = u\}$. When $Gu$ is differentiable at $u$, we denote $T_u(Gu)$ the tangent space of $Gu$ at $u$.

## 2.1 Invariance and Solvability of the Newton Direction

**Lemma 2.1** **(a)** *$\nabla J$ is $\mathcal{G}$-equivariant, i.e., $\nabla J(gu) = g^{-1}\nabla J(u), \quad \forall u \in H, g \in \mathcal{G}$;*

**(b)** *$\nabla J(u) \in H_G$ for any subgroup $G \subset \mathcal{G}$ and $u \in H_G$;*

**(c)** *$\langle J''(u)w, v\rangle = \langle J''(gu)gw, gv\rangle\ \forall u, v, w \in H, g \in \mathcal{G}$, and in particular, $J''(u)(H_G) \subset H_G$ for any subgroup $G \subset \mathcal{G}$ and $u \in H_G$.*

**Proof.** Using the invariance of $J$ we easily get $\langle J'(gu), v\rangle = \langle J'(u), gv\rangle = \langle g^{-1}J'(u), v\rangle$. This shows $\nabla J(gu) = g^{-1}\nabla J(u)$, which implies (a) and (b). Let $G$ be a subgroup of $\mathcal{G}$. To prove (c), differentiating again we have $\langle J''(u)w, v\rangle = \langle J''(gu)gw, gv\rangle$ for all $u, v, w \in H$. For

$u \in H_G$ and $w \in H_G$, we obtain $\langle J''(u)w, v\rangle = \langle g^{-1}J''(u)w, v\rangle$. Thus $J''(u)w = g^{-1}J''(u)w$ for all $g \in G$, and we conclude $J''(u)w \in H_G$, i.e, $J''(u)(H_G) \subset H_G$. ∎

Lemma 2.1 (a) states that if $u^*$ is a critical point, i.e., $\nabla J(u^*) = 0$, then $\nabla J(gu^*) = 0 \ \forall g \in \mathcal{G}$. This implies that when $\mathcal{G}$ has a continuous subgroup $G$ and $u^* \notin H_G$, the continuous orbit $G_{u^*}$ is a critical point set continuous at $u^*$. Thus $u^*$ is not isolated and therefore degenerate, i.e., $\ker(J''(u^*)) \neq \{0\}$. If $G$ is differentiable subgroup of $\mathcal{G}$, we have

**Lemma 2.2** *Let $G$ be a differentiable subgroup of $\mathcal{G}$ and $u \notin H_G$ be a critical point of $J$. Then $T_u(Gu) \subset \ker(J''(u))$. Here $T_u(Gu)$ is the tangent space of $Gu$ at $u$.*

**Proof.** Let $v \in T_u(Gu)$ and consider a one-parameter curve $\gamma : (-\epsilon, \epsilon) \to Gu$ such that $\gamma(0) = u, \gamma'(0) = v$. Then $J'(\gamma(t)) = 0 \ \forall t \in (-\epsilon, \epsilon)$. For any fixed $w$ let $g : (-\epsilon, \epsilon) \to \mathbb{R}$ be defined by $g(t) = (J'(\gamma(t)), w)$. Then $g'(0) = 0$, but $g'(0) = (J''(u)v, w)$. Since $w$ is arbitrary we have $J''(u)v = 0$. ∎

If $u^*$ is a nondegenerate critical point of $J$, i.e., $\ker(J''(u^*)) = \{0\}$, then $\ker(J''(u)) = \{0\}$ for $u$ close to $u^*$. When the degeneracy of a critical point $u^*$ is caused only by differentiable group actions of $G$, i.e., $\ker(J''(u^*)) = T_{u^*}(Gu^*)$, we must have $u^* \notin H_G$. Thus it is reasonable to assume that for $u$ close to $u^*$ and $u \in H \setminus H_G$, $\ker(J''(u)) \subset T_u(Gu)$ holds. Then we have

**Lemma 2.3** *Let $G$ be a differentiable subgroup of $\mathcal{G}$ and $u \in H \setminus H_G$. If $\ker(J''(u)) \subset T_u(Gu)$, then equation (1.3) is always solvable.*

**Proof.** If $\nabla J(u) = 0$, it is obvious. Let $v \in T_u(Gu)$ and consider a one-parameter curve $\gamma : (-\epsilon, \epsilon) \to Gu$ such that $\gamma(0) = u, \gamma'(0) = v$. Let $g(t) = J(\gamma(t))$. Then $g'(0) = 0$ due to the invariance of the functional $J$. Since $g'(0) = (\nabla J(u), v)$, we have $\nabla J(u) \perp T_u(Gu)$ and therefore $\nabla J(u) \perp \ker(J''(u))$ when $\ker(J''(u)) \subset T_u(Gu)$. So (1.3) is always solvable. ∎

The above result implies that the Newton direction $\nu$ of $J$ at $u$ can be solved from (1.3) instead of the much more complicated problem (1.2) when $u$ is close to a critical point $u^*$ whose degeneracy is caused only by a differentiable subgroup actions of $G$. Can Equation (1.3) be uniquely solved? Will the Newton direction $\nu$ of $J$ at $u$ have the same symmetry as that of $u$? These two uniqueness and invariance problems are actually closely related.

**Lemma 2.4** *Let $G$ be a subgroup of $\mathcal{G}$ and $u \in H_G$. If $w \in H$ is a solution to (1.3), then $w_G \in H_G$ is a solution of (1.3) where $w_G = \int_G g(w)dg$ is the Haar projection of $w$ onto $H_G$. Thus the Newton direction is always in $H_G$. Furthermore, if (1.3) is uniquely solvable in $H_G$, then $w_G$ is the Newton direction.*

**Proof.** Since $\nabla J(u) \in H_G$ by Lemma 2.1 (b) and $w_G \in H_G$ by the Haar projection, we only have to prove that $w_G$ is a solution to (1.3). By Lemma 2.1 (c), we have

$$\langle \nabla J(u), v \rangle = \langle J''(u)w, v \rangle = \langle J''(gu)gw, gv \rangle \; \forall v \in H, g \in \mathcal{G}.$$

Taking $v \in H_G$ and $g \in G$, we obtain $\langle J''(gu)gw, gv \rangle = \langle J''(u)gw, v \rangle$. Thus

$$\langle J''(u)gw - \nabla J(u), v \rangle = 0 \quad \text{or} \quad (J''(u)gw - \nabla J(u)) \perp H_G \; \forall g \in G.$$

Since the Haar integral is linear and normalized, and $\nabla J(u) \in H_G$, it follows that

$$\int_G (J''(u)gw - \nabla J(u))\, dg = (J''(u)w_G - \nabla J(u)) \perp H_G$$

as well. Then by Lemma 2.1 (c), $w_G \in H_G$ implies $J''(u)w_G - \nabla J(u) \in H_G$. We must have $J''(u)w_G - \nabla J(u) = 0$. When (1.3) is solvable, the Newton direction $\nu$ must be a solution to (1.3). It has been shown in [27] that the Haar projection $\nu_G$ of $\nu$ is the orthogonal projection of $\nu$ onto $H_G$ and $\nu_G$ is also a solution to (1.3) by the previous part. We have $\|\nu_G\| \leq \|\nu\|$ and the equality holds if and only if $\nu \in H_G$.

If (1.3) is uniquely solvable in $H_G$, which means for all solutions $w$ of (1.3), their orthogonal projections $w_G$ onto $H_G$ are the same, then $w_G$ is the Newton direction. ∎

We conclude here that finding $w_G$ by the Haar projection is equivalent to solving the least-norm solution to the linear system (1.3).

## 2.2 Implementation of Newton Method

Let $G$ be a differentiable subgroup of $\mathcal{G}$ and $u^* \in H \setminus H_G$ be a critical point to be found whose degeneracy is created only by the group actions of $G$. Thus $u^* \in H_{\mathcal{G}_{u^*}}$. Assume[1] each $u \in H_{\mathcal{G}_{u^*}}$ is an isolated point in $H_{\mathcal{G}_{u^*}} \cap Gu$. Thus the degeneracy caused by the group actions of $G$ does not take place in $H_{\mathcal{G}_{u^*}}$. It follows that the equation $J''(u)\nu = v$ has a unique solution $\nu$ in $H_{\mathcal{G}_{u^*}}$ for all $u, v \in H_{\mathcal{G}_{u^*}}$. Therefore the uniqueness and invariance problems can be solved by confining our problem to the subspace $H_{\mathcal{G}_{u^*}}$. This implies that we have to enforce the symmetries defined by the isotropy subgroup $\mathcal{G}_{u^*}$. For numerical implementation, it can be easily done as follows.

Choose an initial guess $u_0 \in H_{\mathcal{G}_{u^*}}$ close to $u^*$, (such $u_0$ has the same symmetry as that of $u^*$). This can be done by the local minimax method due to its invariance to symmetries

[1]For most applications this assumption will be satisfied.

(see [27]). Then by Lemma 2.1, $J'(u_0) \in H_{\mathcal{G}_{u^*}}$ and the equation (1.3) or $J''(u_0)\nu = J'(u_0)$ has a unique solution $\nu_0 \in H_{\mathcal{G}_{u^*}}$ which can be found through solving (1.3) for the least-norm solution. The updated solution $u_1 = u_0 - s_0 v_0 \in H_{\mathcal{G}_{u^*}}$ where $s_0 > 0$ is a stepsize determined by, e.g., Armijo's rule, has the same symmetry as that of $u_0$. Thus the symmetry of $u_0$ is preserved and passed to $u_1$ and we can continue this way to obtain the uniqueness and invariance of the Newton direction in $H_{\mathcal{G}_{u^*}}$. The local convergence of the generalized Newton method is then applied. When numerical error is considered, to overcome the symmetric degeneracy problem, in general, the Haar projection is needed to ensure the solvability of (1.3). The following example is of instructional.

**Example 2.1** Let $J(x,y) = \frac{1}{2}(x^2+y^2) - \frac{1}{4}(x^2+y^2)^2$. Then

$$J'(x,y) = \begin{bmatrix} x(1-(x^2+y^2) \\ y(1-(x^2+y^2)) \end{bmatrix}, \; J''(x,y) = \begin{bmatrix} 1-2x^2-(x^2+y^2) & -2xy \\ -2xy & 1-2y^2-(x^2+y^2) \end{bmatrix},$$

$$\det(J''(x,y)) = (1-(x^2+y^2))(1-3(x^2+y^2)).$$

Thus $(0,0)$ is the local minimum type critical point and $(x_s, y_s)$ with $x_s^2+y_s^2 = 1$ are the saddle points. Let $\mathcal{G} = \mathbb{O}(2) = \mathbb{Z}_2 \times \mathbb{S}^1$ where $\mathbb{O}(2)$ is the group of all $2\times 2$ orthogonal matrices, $\mathbb{Z}_2$ is generated by the matrix $\left[\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right]$ and $\mathbb{S}^1$ is the group of all matrices $\left[\begin{smallmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{smallmatrix}\right]$, $0 \le \theta < 2\pi$. Thus the subgroup $\mathbb{Z}_2$ represents the reflection about the line $x = y$ and the subgroup $\mathbb{S}^1$ represents all rotations. The subgroup $G = \mathbb{S}^1$ is differentiable and creates degeneracy of a critical point not in $H_G$. We have $(0,0) \in H_G$ and $(x_s, y_s) \notin H_G$. It is clear that $(0,0)$ is a nondegenerate critical point with $\det(J''(0,0)) = 1$ and all the saddle points $(x_s, y_s)$ are degenerate. For each $u = (x_s, y_s)$, $Gu = \{(x,y) : x^2+y^2 = 1\}$ and $T_u(Gu) = \{(x,y) : x_s x + y_s y = 0\} = \{(x, -\frac{x_s x}{y_s}) : x \in \mathbb{R}\}$. By Lemma 2.2, $T_u(Gu) \subset \ker(J''(x_s, y_s))$. Indeed we have $J''(x_s,y_s)(x, -\frac{x_s x}{y_s})^T = (0,0)^T$.

Although for all $(x,y)$ with $x^2+y^2 \neq 1, \frac{1}{3}$, $J''(x,y)$ is invertible, the condition number of the matrix $J''(x,y)$ gets worse as $(x,y) \to (x_s, y_s)$. The usual Newton method will fail to provide any reliable solution. If we consider the saddle point $u^* = (\frac{\sqrt{2}}{2}, \frac{\sqrt{2}}{2})$, the isotropy subgroup at $u^*$ is $\mathbb{Z}_2$. The corresponding invariant subspace is $H_{\mathbb{Z}_2} = \{(x,y)^T\}$ such that $\left[\begin{smallmatrix} x \\ y \end{smallmatrix}\right] = \left[\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right] \left[\begin{smallmatrix} x \\ y \end{smallmatrix}\right]$, i.e., $H_{\mathbb{Z}_2} = \{(x,x)^T\}$. By confining the problem in the subspace $H_{\mathbb{Z}_2}$, we have $J(x) = x^2 - x^4$, $J'(x) = 2x(1-2x^2)$ and $J''(x) = 2(1-6x^2)$. At the saddle point $x = \frac{\sqrt{2}}{2}$, $J''(\frac{\sqrt{2}}{2}) = -4$ is invertible. In implementation, for each $u = (z,z)^T \in H_{\mathbb{Z}_2}$, we have $H_{\mathbb{Z}_2} \cap Gu = \{u, -u\}$. Thus $G$ will not cause any degeneracy in $H_{\mathbb{Z}_2}$. With $J'(z,z) =$

$(z(1-2z^2), z(1-2z^2))^T \in H_{\mathbb{Z}_2}$, the equation $J''(z,z)(x,y)^T = J'(z,z)$ has a unique solution $(x,y) \in H_{\mathbb{Z}_2}$ where $x = y = \frac{z(1-2z^2)}{1-6z^2}$ and $-\frac{\sqrt{6}}{6} < z < \frac{\sqrt{6}}{6}$.

## 2.3 Insensitivity of Invariance of Newton's Method to Numerical Error

In [27], the invariance of the local minimax method to a symmetry is proved, i.e., if an initial guess $u_0$ is chosen in an invariant subspace $H_G$ under a subgroup $G \subset \mathcal{G}$, then the sequence generated by the algorithm will remain in $H_G$. However, such an invariance is sensitive to numerical error in computing saddle points, because it searches a saddle point through a min-max method. The minimization process keeps $J$ strictly descending along the sequence $\{u_k\}$ generated by the algorithm. To see the significant differences, let $u_k \in H_G$ be a point closed to a saddle point $u^* \in H_G$. Thus $\nabla J(u_k)$ is small, the numerical errors in computing $\nabla J(u_k)$ dominate the symmetry of $\nabla J(u_k)$. This leads to $u_{k+1} \in H \setminus H_G$. For the minimax method, since $u^*$ is a saddle point, the minimization search finds a slider (a descent direction) outside $H_G$ away from $u^*$. Then $\|\nabla J(u_{k+1})\|$ increases and the asymmetric part of $\nabla J(u_{k+1})$ gets larger. Consequently the invariance of the sequence $\{u_k\}$ collapses and the search fails to reach $u^*$. The Haar projection has to be used (See [7,27]) to preserve the symmetry of $\nabla J(u_k)$. In contrast to the local minimax method, the Newton method does not assume or use a variational structure. It finds a local minimum point $u^*$, not a saddle point, of $\|\nabla J(u)\|$. Once $u_k$ is in a local basin of $\|\nabla J(u)\|$ around $u^*$, due to Armijo's rule, it keeps $\|\nabla J(u_k)\|$ strictly descending. Although $u_{k+1} \in H \setminus H_G$, $\|\nabla J(u_{k+1})\|$ is closer to 0. Thus $u_{k+1}$ is still in the local basin around $u^*$ and is a better approximation to $u^* \in H_G$. The asymmetric part of $u_k$ will be kept within the norm of the numerical errors. In conclusion, the invariance of the Newton method is insensitive to numerical errors, therefore the Haar projection (an averaging formula) as suggested and used for the local minimax method in [27] is not necessary for the Newton method to preserve a symmetry.

The insensitivity of the invariance of the Newton method to numerical errors is double-edged. If one knows the symmetry of a solution $u^*$ to be found, then it is of advantageous. One can choose an initial guess $u_0$ with the same symmetry of $u^*$ to obtain an easy implementation for finding the Newton direction and preserve its invariance. Otherwise, it becomes a trap, when an initial guess $u_0$ has a symmetry different from that of $u^*$, the whole sequence generated by the Newton method will be trapped in the invariant subspace defined by the symmetry of $u_0$ and fails to reach $u^*$.

When a symmetry is associated with a continuous group $G$ of actions, it causes degeneracy and the corresponding Haar projection is an integral over $G$ and very difficult to compute. To overcome the symmetric degeneracy problem with numerical error, the Haar projection is needed in general. However, in many applications such as the examples in Section 4, such a symmetric degeneracy is removable when a discretization is used, because after a discretization, $G$ is approximated by a finite group. The truncation error is unpredictable, but it is in a much high order than the discretization error, which actually makes (1.3) more solvable. The above analysis suggests that in this case, the Haar projection is not needed to overcome the symmetric degeneracy problem with numerical error. Thus the Newton method can be used not only to speed up convergence but also to avoid using the Haar projection. This leads to the following *local minimax-Newton algorithm.*

## 2.4 A Local Minimax-Newton Algorithm

**Step 1:** Given $\varepsilon_M > \varepsilon_N > 0$ and $n-1$ previously found critical points $w_1, \ldots, w_{n-1}$, of which $w_{n-1}$ has the highest critical value. Set the support space $L = \text{span}\{w_1, \ldots, w_{n-1}\}$. Let $v^1 \in L^\perp$ be an ascent direction at $w_{n-1}$. Let $t_0^0 = 1$, $v_L^0 = w_{n-1}$ and set $k = 0$;

**Step 2:** Using the initial guess $w = t_0^k v^k + v_L^k$, solve for $w^k = \arg \max_{u \in [L, v^k]} J(u)$ and denote $w^k = t_0^k v^k + v_L^k$ where $t_0^k, v_L^k$ have been updated;

**Step 3:** Compute the negative gradient $d^k = -\nabla J(w^k)$;

**Step 4:** If $\|d^k\| \leq \varepsilon_M$ then set $w^0 = w^k$, k=0 and goto Step 7; else goto Step 5;

**Step 5:** Set $v^k(s^k) = \frac{v^k + s^k d^k}{\|v^k + s^k d^k\|}$ where $s^k$ satisfies certain stepsize rule (See [15, 16]);

**Step 6:** Set $v^{k+1} = v^k(s^k)$ and update $k = k + 1$ then goto **Step 2**;

**Step 7:** Solve $J''(w^k)\nu = J'(w^k)$ for the least-norm solution $\nu^k$;

**Step 8:** Set $w^{k+1} = w^k - s^k \nu^k$ where $s^k$ satisfies, e.g., the Armijo's rule (1.1);

**Step 9:** Compute the gradient $\nabla J(w^{k+1})$;

**Step 10:** If $\|\nabla J(w^{k+1})\| < \varepsilon_N$ then output $w^{k+1}$ and stop; else set $k = k + 1$, goto **Step 7**.

Steps 1-6 represent the local minimax method [15, 16] to locate an initial guess that is sufficiently close to a desirable saddle point and Steps 7-10 represent the Newton method described in this paper to speed up the convergence.

When a symmetry is involved in a saddle point $u^*$ to be found, we

(1) identify the symmetry of $u^*$ by defining an invariant subspace $H_G$. Let $L_G = L \cap H_G$ and replace $L$ by $L_G$ in the algorithm; In many cases, such as those examples in Section 3, we have $L_G = \{0\}$;

(2) Choose an initial guess $v^1 \in H_G$;

(3) Do iterations from Step 2 to Step 6.
**Case 1.** If we do not want to enforce the symmetry, we should choose $\varepsilon_M = 10\varepsilon$ where $\varepsilon$ represents the order of the numerical error in computing $\nabla J(w^k)$, e.g., $\varepsilon = 10^{-2}$. Since the minimax method is invariant to a symmetry, when $\|\nabla J(w^k)\| > \varepsilon_M$, the symmetry of $\nabla J(w^k)$ still dominates the numerical error in $\nabla J(w^k)$. Usually the numerical error starts to dominate the symmetry of $\nabla J(w^k)$ when $\|\nabla J(w^k)\|$ is close to $\varepsilon$;
**Case 2.** If we want to enforce the symmetry, we only have to change Step 3 as $d^k = -\mathcal{H}(\nabla J(w^k))$ where $\mathcal{H}$ is the Haar projection defined in Lemma 2.4. In this case, we can choose $\varepsilon_M = 10\varepsilon$ or smaller.

(4) For Steps 7-10, if a degeneracy caused by a continuous group $G$ of actions is removable by a discretization, then no Haar projection is needed, otherwise do the Haar projection.

# 3 Applications to Semilinear Elliptic Equations

## 3.1 Problems and setting-up

The model equation we look at is the following semilinear elliptic equation

$$\begin{cases} -\Delta u(x) = f(x, u(x)), & \text{in } \Omega \\ u = 0, & \text{on } \partial\Omega, \end{cases} \tag{3.1}$$

where $\Omega \subset \mathbf{R}^N$ is bounded, $f$ is a $C^1$ function satisfying certain growth and regularity conditions [23] and we seek weak solutions in $H = W_0^{1,2}(\Omega)$. The energy functional is

$$J(u) = \int_\Omega \{\frac{1}{2}|\nabla u(x)|^2 - F(x, u(x))\}\, dx \quad \text{where} \quad F(x,t) = \int_0^t f(x,\tau) d\tau. \tag{3.2}$$

Then critical points of $J(u)$ correspond to weak solutions of equations (3.1). Problems of this type appear as models in many applied areas. Mathematically, people have been interested in understanding the solution structures in terms of existence and non-existence, the number of solutions as well as in obtaining qualitative property of solutions such as the geometric, symmetric and nodal properties. Though great progress has been made still many important open questions remain unsettled. Here, we are mainly concerned in uncovering new phenomena by numerically examining the qualitative behavior of both positive solutions and nodal solutions of this type of elliptic boundary value problems. For $u, w \in H$, we have

$$\langle J'(u), w\rangle_{H^*\times H} = \frac{d}{dt}|_{t=0} J(u+tw) = \int_\Omega \nabla u \nabla w - f(x, u(x))w\, dx.$$

Thus $d = \nabla J(u) = u - (-\Delta)^{-1} f(x, u) \in H$. Taking the second derivative, we have

$$\langle J''(u)\nu, w\rangle = \frac{d}{dt}|_{t=0}\langle J'(u+t\nu), w\rangle = \int_\Omega \nabla \nu \nabla w - f'_u(x, u(x))\nu w\, dx, \quad \forall \nu \in H,$$

which implies that $J''(u) = I - (-\Delta)^{-1} f'_u(\cdot, u)$. Under standard conditions [23] on $f$, $(-\Delta)^{-1} f'_u(\cdot, u)$ is a compact operator and $J''(u)$ is a Fredholm operator with index zero. By setting $\langle J'(u), w\rangle = \langle J''(u)\nu, w\rangle$ for all $w \in H$, the Newton direction $\nu$ as defined in (1.3) can be obtained from weakly solving

$$\begin{cases} -\Delta\nu(x) - f'_u(x, u(x))\nu(x) = -\Delta u(x) - f(x, u(x)), & x \in \Omega, \\ \nu(x) = 0, & x \in \partial\Omega. \end{cases} \tag{3.3}$$

**Remark 3.1** (a) Newton's method has been applied to variational problems in the literature usually by solving a discretized Euler-Lagrange equation. This approach requires to solve for $J'(u)$ and $J''(u)$, then compute $\nu = (J''(u))^{-1}J'(u)$, or, $\nu = (J''(u))^{\dagger}J'(u)$ when $J''(u)$ is not invertible, and therefore is much more computationally expensive and difficult. While solving the Newton direction $\nu$ directly from (3.3) is much simpler and less expensive. In many cases when $J''(u)$ is not invertible, $\nu$ is still solvable from (3.3), such as the case where the singularity of $J''(u)$ is caused only by a continuous group of actions.
(b) When an initial guess $u_0$ and its Laplacian $\Delta u_0$ are given, the Newton direction $\nu_0$ is solved from (3.3) and $s_0$ is determined by, e.g., the Armijo rule. Then $u_1 = u_0 - s_0\nu_0$ and $\Delta u_1 = \Delta u_0 - s_0\Delta\nu_0$ where $\Delta\nu_0(x) = \Delta u_0(x) + f(x, u_0(x)) - f'_u(x, u_0(x))\nu_0(x)$ is known. Thus no computation of the Laplacian of the updated numerical solution $u_1$ is required.

## 3.2 Numerical Examples

In this section, we apply the local minimax method (MM), the Newton method (NM) and the local minimax-Newton method (MM+NM) to numerically solve the Henon equation

$$(3.4) \qquad \begin{cases} -\Delta u(x) = |x|^q u^3(x) & \text{in } \Omega, \\ u(x) = 0 & \text{on } \partial\Omega \end{cases}$$

for multiple solutions in $H = H_0^1(\Omega)$ where $\Omega$ is either the unit disk or an annulus. We are interested in finding new phenomena in symmetry breaking and nodal property of solution structure. The symmetries of the problem can be described by the group actions $\mathcal{G} = \mathbb{O}(2) = \mathbb{Z}_2 \times \mathbb{S}^1$ where $\mathbb{O}(2)$ is the set of all 2 by 2 orthogonal matrices, $\mathbb{Z}_2$ and $\mathbb{S}^1$ represent, respectively, the reflection about the x-axis and all the rotations. For $u \in H$, $g \in \mathbb{S}^1$ and the generator $\bar{h} \in \mathbb{Z}_2$, we define $g(u)(x) = u(gx)$, $h(u)(x) = \pm u(\bar{h}x)$, where +1 and -1 represent, respectively, the even and the odd reflection, and the odd reflection is applicable if an even n-rotationally symmetry is considered. Then $\mathcal{G}$ becomes a compact Lie group that acts isometrically on $H$ and $G = \mathbb{S}^1$ is a differentiable subgroup that creates degeneracy for a critical point $u^* \notin H_G$, i.e., $u^*$ is radially asymmetric (or non-radial).

For a radially asymmetric but n-rotationally symmetric solution $u^*$, the isotropy subgroup of $\mathcal{G}$ at $u^*$ is $\mathcal{G}_{u^*} = \{\mathrm{Id}, h^i g_i, i = 0, 1, ..., n-1\}$ where $g_i = \begin{bmatrix} \cos\theta_i & \sin\theta_i \\ -\sin\theta_i & \cos\theta_i \end{bmatrix}$, $\theta_i = i\dfrac{2\pi}{n}$, $i = 0, 1, .., n-1$. and for each $u \in H_{\mathcal{G}_{u^*}}$, $H_{\mathcal{G}_{u^*}} \cap Gu = \{g_i u, i = 0, 1, ..n-1\}$. Thus the differentiable subgroup $G$ causes no degeneracy in $H_{\mathcal{G}_{u^*}}$. By confining the problem in $H_{\mathcal{G}_{u^*}}$, the Newton direction can be uniquely solved from (3.3) in $H_{\mathcal{G}_{u^*}}$. For implementation, this means that we only need to take an initial guess $u_0$ in $H_{\mathcal{G}_{u^*}}$ and close to $u^*$. In the following numerical examples, $\varepsilon = \|\nabla J(u_k)\|$ and $u_0$ is computed from solving the linear equation

$$(3.5) \quad \begin{cases} -\Delta u_0(x) = c(x), & x \in \Omega, \\ u_0(x) = 0, & x \in \partial\Omega \end{cases} \quad \text{where } c(x) = \begin{cases} +1 & \text{if } u_0 \text{ is concave down at } x \\ -1 & \text{if } u_0 \text{ is concave up a } x \\ 0 & \text{otherwise.} \end{cases}$$

**Case 1:** $\Omega = \{(x_1, x_2) : x_1^2 + x_2^2 < 1\}$.

**(1)** Let $q = 0.5$ in (3.4). It is known that the equation has a unique positive solution which is radially symmetric as shown in Figure 1.

(a) Using an initial guess $u_0$ which is radially asymmetric but symmetric about the x-axis with $c(x_1, x_2) = -1$ if $|(x_1, x_2) - (0.5, 0)| \leq 0.5$ and $c(x_1, x_2) = 0$ otherwise. Then NM failed to converge in 120 iterations and 35 MM iterations yield $\varepsilon < 10^{-4}$. While 6 MM iterations give $\varepsilon < 10^{-1}$ and then followed by 5 NM iterations, it yields $\varepsilon < 10^{-8}$.

(b) Using a radially symmetric initial guess $u_0$ from $c(x_1, x_2) = -1$. Then 5 NM iterations yield $\varepsilon < 10^{-12}$ and 8 MM iterations reach $\varepsilon < 10^{-4}$.

**(2)** Next let $q = 2$ in (3.4). Then the equation has a radially symmetric positive solution and other radially asymmetric positive solutions ([3]). Rotating a radially asymmetric solution for any angle gives a radially asymmetric solution as well. Thus such a solution is degenerate. The radially symmetric positive solution has the highest energy among all the positive solutions. Without using the symmetry, such a solution is extremely elusive to capture.

(a) Using a radially asymmetric initial guess $u_0$ from $c(x_1, x_2) = -1$ if $|(x_1, x_2) - (0.5, 0)| \leq 0.5$ and $c(x_1, x_2) = 0$ otherwise. Then 11 MM iterations get the solution as in Figure 2 with $\varepsilon < 5 * 10^{-3}$ and 7 NM iterations find the same solution with $\varepsilon < 10^{-7}$.

(b) Using an radially symmetric initial guess $u_0$ from $c(x_1, x_2) = -1$. Then 21 MM iterations obtain the solution as in Figure 3 with $\varepsilon < 3 * 10^{-3}$, which is a rotation of the solution in Figure 2 and 4 NM iterations find the radially symmetric solution as in Figure 4 with $\varepsilon < 10^{-7}$. Such a solution cannot be captured by MM without enforcing the symmetry.

(c) Using an initial guess $u_0$ from $c(x_1, x_2) = -\text{sign}(x_1)$. $u_0$ is odd 2-rotation y-axis symmetric. NM failed to converge. Then first 2 MM iterations followed by 8 MM iterations yield a sign-changing solution as in Figure 5 with $\varepsilon < 10^{-7}$. Note that the solution in Figure 5 has the same symmetries as that of the initial guess $u_0$.

(d) To show that the invariance of NM is very insensitive to numerical error, using an initial guess $u_0$ from $c(x_1, x_2) = +1$ if $-\frac{1}{4}\pi < \tan^{-1}(\frac{x_2}{x_1}) < \frac{1}{4}\pi$ or $\frac{3}{4}\pi < \tan^{-1}(\frac{x_2}{x_1}) < \frac{5}{4}\pi$ and $g(x_1, x_2) = -1$ otherwise. $u_0$ is odd 4-rotationally symmetric. The corresponding invariant subspace is much smaller. Again NM failed to converge. First 2 MM iterations followed by 9 NM iterations yield a solution as in Figure 6 with $\varepsilon < 10^{-11}$.

**Case 2:** $\Omega = \{(x_1, x_2) : 0.4 < x_1^2 + x_2^2 < 1\}$ and $q = 2$ in (3.4).

The equation has a radially symmetric and other radially asymmetric positive solutions ([4]). Rotating a radially asymmetric solution for any angle is still a radially asymmetric solution. Thus such a solution is degenerate. The radially symmetric positive solution has the highest energy among all the positive solutions. Without using the symmetry, such a solution is extremely elusive to capture.

(a) Using a radially asymmetric initial guess $u_0$ from $c(x_1, x_2) = -1$ if $|(x_1, x_2) - (0.7, 0)| \leq$

0.3 and $c(x_1, x_2) = 0$ otherwise. Then 17 MM iterations get the solution as in Figure 7 with $\varepsilon < 3 * 10^{-3}$ and 9 NM iterations yield the same solution with $\varepsilon < 10^{-9}$.

(b) Using an initial guess $u_0$ from $c(x_1, x_2) = -1$ if $-\frac{1}{4}\pi < \tan^{-1}(\frac{x_2}{x_1}) < \frac{1}{4}\pi$ or $\frac{3}{4}\pi < \tan^{-1}(\frac{x_2}{x_1}) < \frac{5}{4}\pi$ and $c(x_1, x_2) = 0$ otherwise. $u_0$ is even 2-rotationally symmetric. First 2 MM iterations followed by 6 NM iterations yield a solution as in Figure 8 with $\varepsilon < 10^{-11}$.

(c) Using an initial guess $u_0$ from $c(x_1, x_2) = -1$ if $-\frac{1}{6}\pi < \tan^{-1}(\frac{x_2}{x_1}) < \frac{1}{6}\pi$, $\frac{1}{2}\pi < \tan^{-1}(\frac{x_2}{x_1}) < \frac{5}{6}\pi$ or $-\frac{5}{6}\pi < \tan^{-1}(\frac{x_2}{x_1}) < -\frac{1}{2}\pi$ and $c(x_1, x_2) = 0$ otherwise. $u_0$ is even 3-rotationally symmetric. First 2 MM iterations followed by 7 NM iterations yield a solution as in Figure 9 with $\varepsilon < 10^{-10}$.

(d) Using a radially symmetric initial guess $u_0$ by setting $c(x_1, x_2) \equiv -1$. Then 4 NM iterations yield the radially symmetric solution as in Figure 10 with $\varepsilon < 10^{-7}$. But MM fails to find the solution without enforcing the symmetry.

For all numerical examples in this section, the Matlab PDE Toolbox is used to generate the domains, finite-element meshes and do computations. The Matlab function **assempde** is used to solve (3.3) for the Newton direction. Note that the degeneracy caused by symmetries in the examples is removable when a discretization is used. Since when the disk or annulus is discretized into finite element grids, the continuous subgroup $S^1$ is approximated by a finite subgroup $S^1_n = \{g_i, i = 0, 1, ..., n-1\}$ and the radial symmetry of the problem is approximated by the n-rotationally symmetry. With this approximation, the symmetric degeneracy of the problem is removed. Without a degeneracy, (3.3) is uniquely solvable and yields the Newton direction $\nu$. By our analysis in Section 2, (3.3) is solvable without numerical error and now it is also solvable with numerical error, therefore such an approximation or a refinement of distretization (finte-element grids) should be stable. Thus no Haar projection is needed.

With the local minimax-Newton algorithm, we are able to carry out many numerical investigations for examining the qualitative behavior and finding new phenomena of both positive and nodal solutions of nonlinear elliptic boundary value problems, e.g., the symmetry breaking and bifurcation phenomena, the dependency of solutions on boundary approximation. We will address those new findings in subsequential papers.

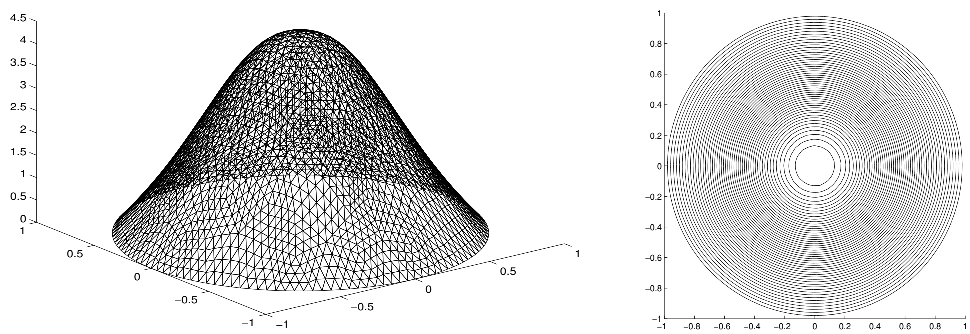

Figure 1: $q = 0.5$. The radially symmetric ground state with $J = 21.5347$.

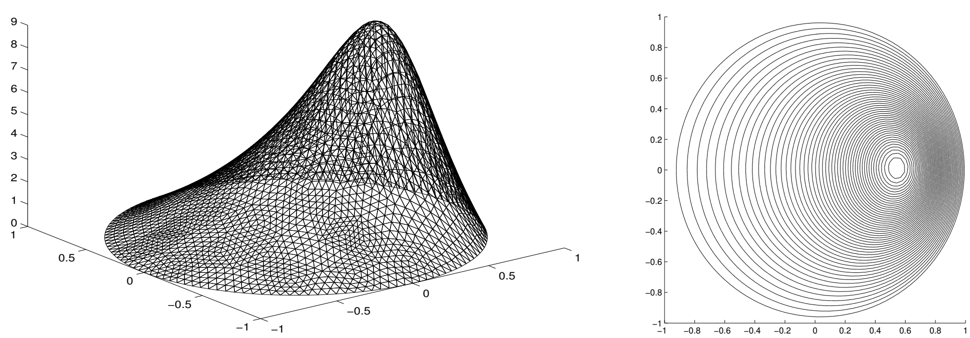

Figure 2: $q = 2$. A radially asymmetric ground state with $J = 70.9280$.

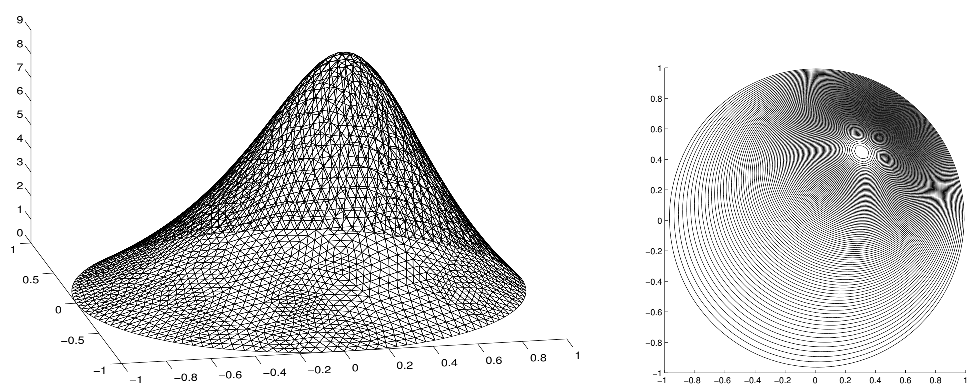

Figure 3: $q = 2$. Another radially asymmetric ground state with $J = 70.8941$.

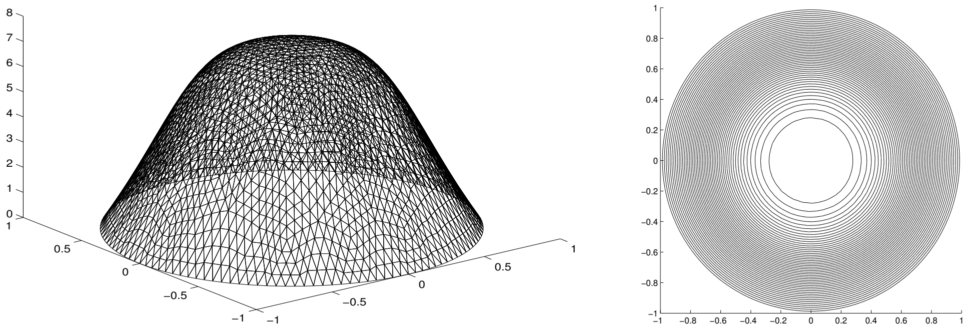


Figure 4: $q = 2$. The radially symmetric solution with $J = 88.1740$.

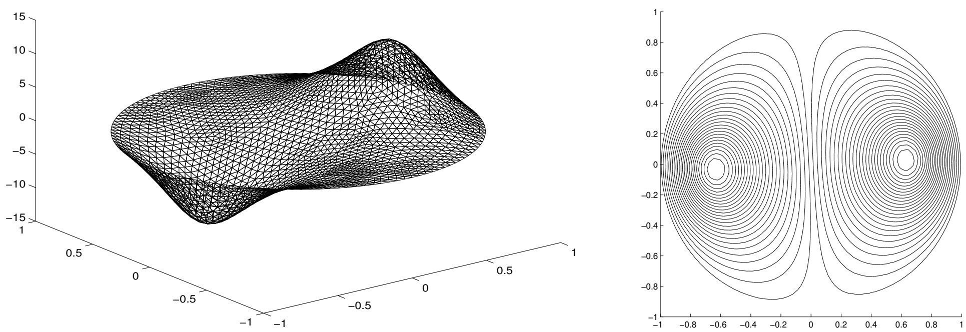


Figure 5: $q = 2$. An odd 2-rotationally symmetric sign-changing solution with $J = 182.9987$.

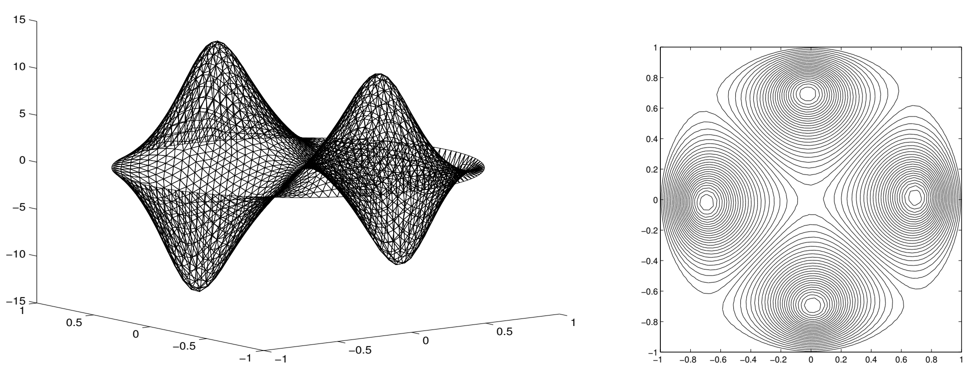


Figure 6: $q = 2$. An odd 4-rotationally symmetric sign-changing solution with $J = 489.2240$.

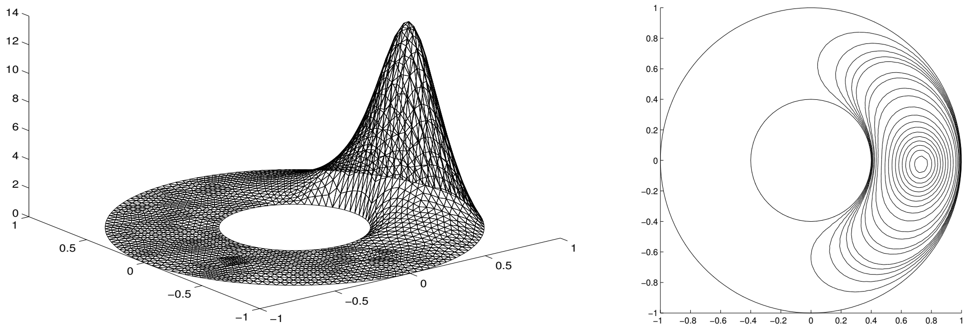


Figure 7: $q = 2$. A radially asymmetric ground state with $J = 143.9674$.

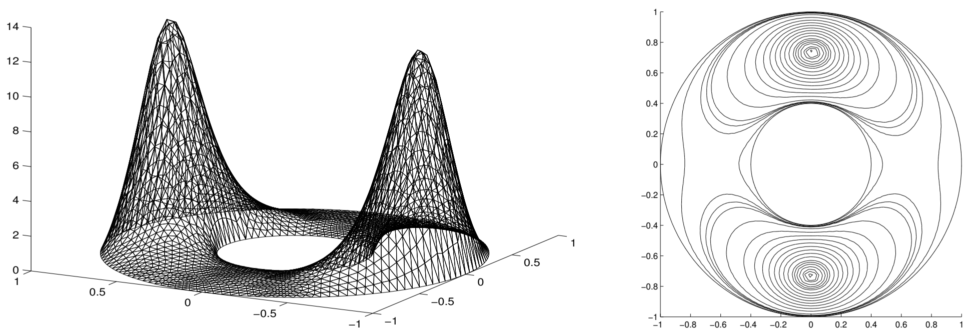


Figure 8: $q = 2$. An even 2-rotationally symmetric solution with $J = 288.5556$.

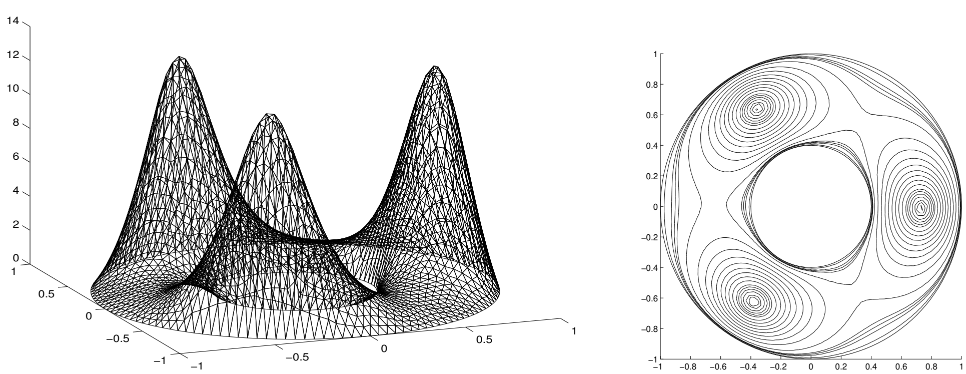


Figure 9: $q = 2$. A 3-rotationally symmetric solution with $J = 429.9529$.

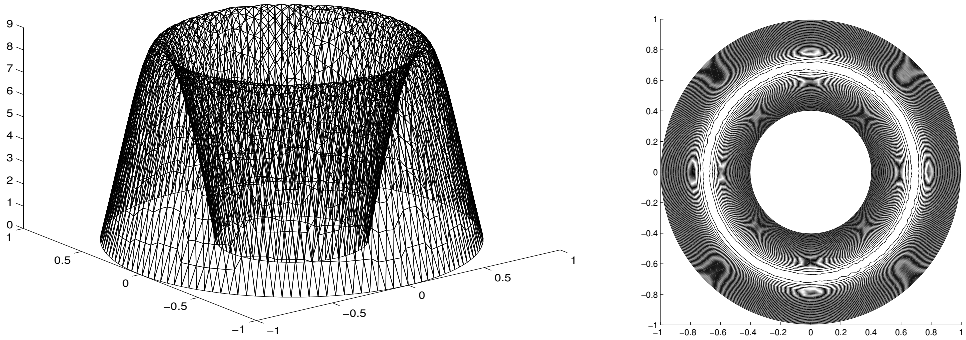

Figure 10: $q = 2$. The radially symmetric solution with $J = 631.9575$.

**Acknowledgment:** The authors wish to thank two anonymous reviewers for their comments which stimulate us for this revision.

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